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Derivation of a continuum model for low temperature plasma flow and its application on arc discharge

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Abstract

A set of governing equations for non-equilibrium plasma flow is derived based on the Boltzmann equation and existing models. This continuum model considers both thermal and chemical non-equilibrium effects and can be applied in a wide range of flow and discharge conditions. The model is verified using a free-burning arc problem, and is applied to investigate the flow and discharge characteristics of an arcjet. It shows that the arc attachment point in arcjet moves downstream with the increasing flow rate due to the arc and flow interaction.

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Keywords: Continuum model; non-equlibrium plasma; CFD; arc discharge.

1. Introduction

Low-temperature plasma flow involves complicated physicochemical process, and has been applied in many applications. Due to the diverse applications, the flow and discharge characteristics of plasma flow may have large variations with different time and spatial scales. Over the past thirty years, numerical simulations have been becoming an active approach to predict the details of the plasma flows. Various sets of governing equations have been employed to model plasma flows in previous studies [1,2]. The derivation of these equations, however, is seldom presented. The validity of the equations is usually covered by the well-accepted fact that plasma flow is hard to be correctly modeled. The present work aims to derive a continuum model for low temperature plasma flow from the Boltzmann equation.

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A typical application is the simulation of arc discharge. Early studies on arc discharge are based on the thermal and chemical equilibrium assumption. Hsu and Pfender [2] first took thermal non-equilibrium effects into consideration in the CFD simulation of a free-burning arc. Haidar [3] later modified the thermal non-equilibrium model by adopting a more reasonable energy exchanging mechanism. Their work adopted the chemical equilibrium assumption and employed the Saha equation to estimate the particle density considering the low flow rate in free-burning. In applications such as arcjet where the time scales of flow and chemical reactions are comparable, chemical non-equilibrium effect has been considered in some CFD modeling [1,4]. The current distribution along the electrode surface, however, was usually preset in simulations.

In this work, a continuum model will be derived based on the Boltzmann equation and existing models. The model will be verified by simulating a free-burning arc problem where measurement data is available. As an application, the model will be employed to simulate the plasma flow of an arcjet. The coupling effects between flow and discharge will be investigated.

2. Continuum model

The statistical behavior of the plasma flow is governed by the Boltzmann equation, which describes the evolution of the velocity distribution function f for each species s in terms of time t and phase space $(\vec{r}, \vec{V})$:

$$\partial_t f_s + \nabla_{\vec{r}} \cdot \left(\vec{V_s} f_s\right) + \nabla_{\vec{V_s}} \cdot \left(\vec{a_s} f_s\right) = C_s, \tag{1}$$

where

$$\vec{a_s} = \frac{\mathbb{Q}_s}{m_s}(\vec{E} + \vec{V_s} \times \vec{B}), \tag{2}$$

C_s is the collision term, $\mathbb{Q}_s$ is species' electric charge, m_s is the molecule weight, $\vec{E}$ and $\vec{B}$ are the electric and magnetic field, respectively. A continuum model can be derived by taking the moments of the Boltzmann equation.

The mass conservation equation for each species is obtained using the zeroth velocity moment:

$$\frac{\partial n_s}{\partial t} + \frac{\partial}{\partial x_i}\left(U_{si} n_s\right) = S_s, \tag{3}$$

where n_s is the number density, S_s is the mass production rate due to chemical reactions, U_{si} is the average velocity. In continuum models, the species velocity is usually expressed as the sum of the average convection velocity u_i and its diffusion velocity u_{si}. The average convection velocity is the mass weighted velocity, thus contribution from electrons is neglected.

$$u_i = \frac{\sum_{s \neq electron} U_{si} n_s m_s}{\sum_{s \neq electron} n_s m_s}. \tag{4}$$

The drift velocity can be derived using the Chapman-Enskog expansion [5,6], which is complicated. The drift diffusion assumption is therefore employed for engineering applications:

$$u_{si} = \frac{\mathbb{Q}_s}{m_s \nu_s}\left(E_i + \varepsilon_{ijk} u_j B_k\right) - \frac{kT}{m_s \nu_s}\frac{\nabla n_s}{n_s}, \tag{5}$$

where k is the Boltzmann constant and ν_s is the elastic collision frequency of specie s.

The overall mass conservation equation is then obtained by summing all the species' equation:

$$\sum_{s \neq electron}\left(\frac{\partial m_s n_s}{\partial t} + \frac{\partial}{\partial x_i}\left(U_{si} n_s m_s\right)\right) = \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}\left(\rho u_i\right) = 0, \tag{6}$$

where ρ is the mass density. Again, the contribution of electron production is neglected because the electron mass is negligible.

Similarly, the momentum equation is derived by integrating the first velocity moment of the Boltzmann equation and summing over all heavy species.

$$\frac{\partial}{\partial t}(\rho u_i)+\frac{\partial}{\partial x_j}(\rho u_i u_j)=-\frac{\partial p}{\partial x_i}+\frac{\partial \tau_{ij}}{\partial x_j}+\left(\sum_{s\neq electron}\sigma_s\right)E_i+\varepsilon_{ijk}\left(\sum_{s\neq electron}j_{sj}\right)B_k+C_{mi}, \tag{7}$$

where p is the pressure contributed from all heavy species, σ_s is the charge density, j_{sj} is the component of electric current due to particle motion:

$$p=\sum\nolimits_{s\neq electron}n_s kT, \tag{8}$$

$$\sigma_s=n_s\mathbb{Q}_s, \tag{9}$$

$$j_{sj}=\left(u_j+u_{sj}\right)n_s\mathbb{Q}_s, \tag{10}$$

The third and fourth terms on the right hand side are the body force terms. The fifth term is the momentum exchange between heavy particles and electrons due to elastic collisions. Graille proved that if $\sqrt{m_e/m_h}$ (m_h is the molecule weight of heavy particles) is at the same order with the Knudsen number when the Chapman-Enskog expansion is employed [7], C_{mi} can be expressed as:

$$C_{mi}=-\frac{\partial p_e}{\partial x_i}+\sigma_e E_i+\varepsilon_{ijk}J_{ej}B_k. \tag{11}$$

The energy conservation equation of electrons is derived by integrating the second velocity moment of the Boltzmann equation. As the energy is directly related to the temperature ($e_e=3kT_e/2m_e$), the equation is expressed in terms of the electron temperature,

$$\frac{5}{2}\frac{\partial}{\partial t}\left(n_e kT_e\right)+\frac{5}{2}\frac{\partial}{\partial x_i}\left(n_e kT_e\cdot\left(u_i+u_{ei}\right)\right)=-\frac{\partial}{\partial x_i}\left(q_{ei}\right)+\frac{Dp_e}{Dt}+J_{ei}(E_i+\varepsilon_{ijk}u_jB_k)+\sum_{r=elec}\varepsilon_r q_r-\sum_{r=elastic}\varepsilon_r q_r, \tag{12}$$

where

$$J_{ej}=u_{ej}n_e\mathbb{Q}_e. \tag{13}$$

The third term on the right hand side is the Joule heating due to body force on electrons. q_{ei} is the heat flux due to electron's thermal motion, which can be approximated using the Fick's Law:

$$q_{ei}=k_e\frac{\partial T_e}{\partial x_i}, \tag{14}$$

$\sum_{r=elec}\varepsilon_r q_r$ is the electron energy loss due to electron induced reactions, which is assumed that electrons provide the energy. $\sum_{r=elastic}\varepsilon_r q_r$ is the energy transferred from electrons to heavy particles due to elastic collision, which is approximated as [7,8]:

$$\sum_{r=elastic}\varepsilon_r q_r=2\frac{m_e n_e}{m_s}\left(\frac{3}{2}T_e-\frac{3}{2}T\right)\cdot\left(\sum_{s\neq electron}\nu_{es}\right)+\sum_{s\neq electron}\left(m_e n_s\nu_{es}\left(u_i+u_{si}\right)\left(u_{si}-u_{ei}\right)\right), \tag{15}$$

where, v_{es} is the collision frequency between species s and electrons, which can be further approximated using the Krook operator [8]. The two terms in Eq. (16) represent energy transfer due to thermal non-equilibrium and friction, respectively.

The temperature equation for heavy particles can be derived in a similar manner. If the temperatures of all heavy species are assumed to be the same, then we have:

$$C_p\left(\frac{\partial \rho T}{\partial t}+\frac{\partial}{\partial x_i}(\rho u_i T)\right)=\frac{\partial}{\partial x_i}\left(\lambda\frac{\partial}{\partial x_i}T\right)-\sum_s\left(\rho_s u_{si} C_{ps}\frac{\partial}{\partial x_i}T\right)+\Phi+\frac{Dp}{Dt}+J_{ion\_i}(E_i+\varepsilon_{ijk}u_j B_k)+\sum_{r=non\_elec}\varepsilon_r q_r+\sum_{r=elastic}\varepsilon_r q_r \cdot \tag{16}$$

The first term on the right hand side is the heat flux term where the Fick's Law is again adopted. The second term is due to mass diffusion. The third term is due to viscous dissipation. The fifth term is the Joule heating due to body force on ions. The sixth term accounts for the heat release due to chemical reactions among heavy species, and the last term is the energy transferred from electrons through elastic collisions.

With regard to electromagnetic fields, the Maxwell equations are always employed. If the quasi-neutral assumption is adopted in arc simulations, the Maxwell equations degenerate into the general Ohm's law.

3. Arc discharge simulation

The derived continuum model is applied to simulate the arc discharge. As a first example, the free-burning arc is simulated, which is used to verify the model and implementation. The reaction mechanism and transport properties follow the setup in Ref. [9]. A comparison between the simulated gas temperature and measurement data is presented in Fig. 1, which shows that the agreement is encouraging. Figure 2 illustrates the gas and electron temperatures. It appears that the difference between the two temperatures becomes significant when approaching to the arc fringe, although thermal equilibrium is achieved in the central region of the arc. This non-equilibrium behavior is consistent with the previous work [2].

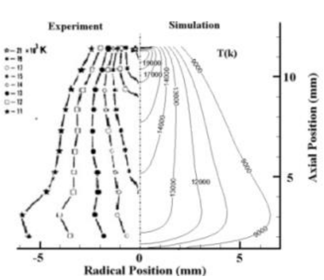

Fig. 1. Comparison with experiment (gas temperature).

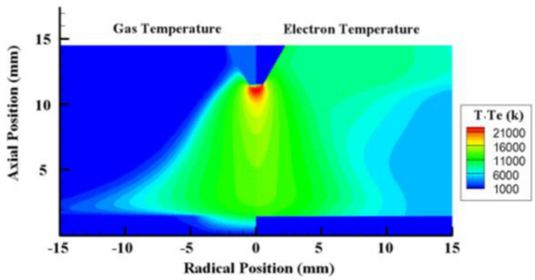

Fig. 2. Comparison between electron and gas temperatures.

Arcjet is a typical application of arc discharge where the discharge and flow is coupled closely. Figure 3 illustrates the schematic of a NASA device [10]. During its operation, the arc heats the passing argon in the constrictor through Joule heating, and the heated gas is accelerated in the expansion nozzle, which produces the thrust. Figure 4 shows the mass flux and current density along the radial direction at a constrictor position of 1.5mm. As the electric current is small near the anode surface, the gas is seldom heated near the wall and thus a large part of gas passes through the constrictor along the wall. As the cold gas is almost insulated, it compresses the electro-conductive arc away from the anode. It seems that the location of maximum mass flux moves away from the wall when the flow rate increases from 140mg/s to 270mg/s. The wider cold gas layer also pushes the arc attachment location downstream, which is illustrated in Fig 5 where the current density and current streamlines are plotted.

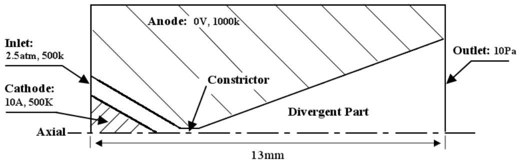

Fig. 3. Schematic of the arcjet.

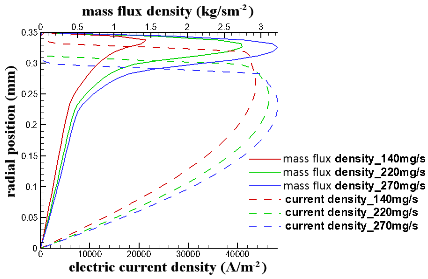

Fig. 4. Mass flux and electric current density along radial position (z=1.5mm)

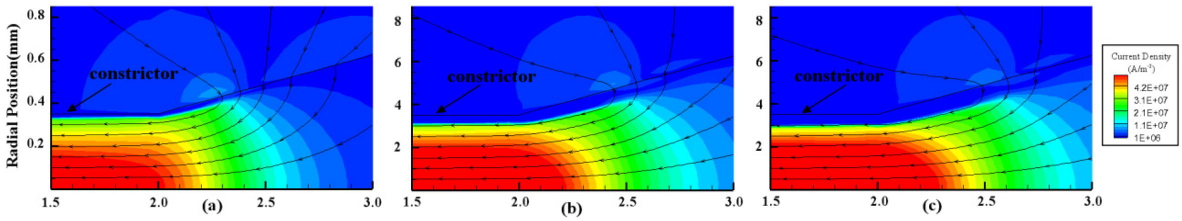

Fig. 5. Current density and current streamlines in the constrictor region under different flow rate (a) 140mg/s; (b) 220mg/s; (c) 270mg/s.

4. Conclusions

In the present study, a non-equilibrium continuum model for plasma flow is derived from the Boltzmann equation. This set of governing equations has been employed to study the flow and discharge characteristics of a free-burning arc and an arcjet. Simulations show that the continuum model predicted correctly the non-equilibrium phenomena associated with the low-temperature plasma flow. Particularly the arc attachment point in arcjet moves downstream with the increasing flow rate due to the arc and flow interaction.

Acknowledgements

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